



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2017 – 10:19 AM EST

PDB ID : 4AI6
Title : Dynein Motor Domain - ADP complex
Authors : Schmidt, H.; Gleave, E.S.; Carter, A.P.
Deposited on : 2012-02-08
Resolution : 3.40 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20029077
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029077

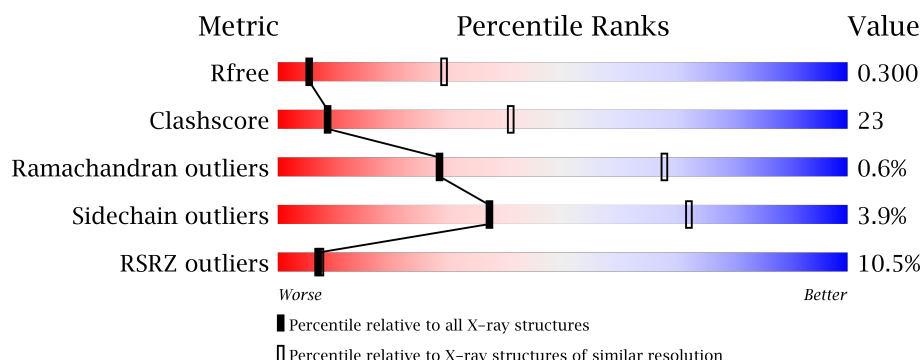
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1679 (3.50-3.30)
Clashscore	112137	1832 (3.50-3.30)
Ramachandran outliers	110173	1789 (3.50-3.30)
Sidechain outliers	110143	1789 (3.50-3.30)
RSRZ outliers	101464	1709 (3.50-3.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	2695	<div> <div>11%</div> <div>66%</div> <div>31%</div> <div>..</div> </div>
1	B	2695	<div> <div>9%</div> <div>67%</div> <div>30%</div> <div>..</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ATP	B	5400	-	-	X	-
3	ADP	A	5401	-	-	X	-
3	ADP	A	5402	-	-	X	-
3	ADP	B	5402	-	-	X	-
4	SO4	A	5403	-	-	X	-
4	SO4	B	5403	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 41678 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

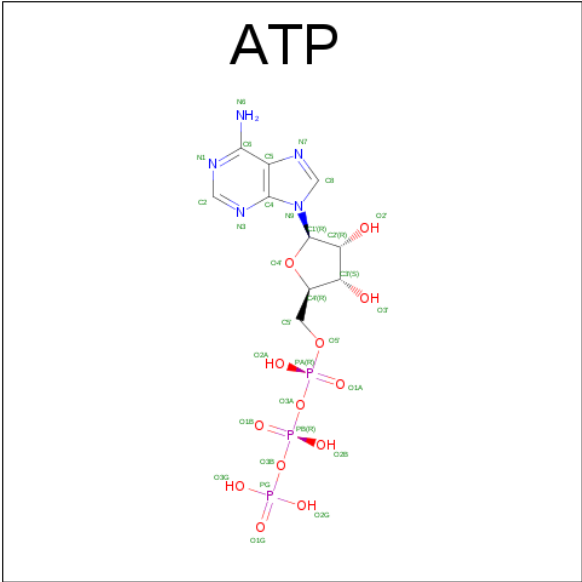
- Molecule 1 is a protein called GLUTATHIONE S-TRANSFERASE CLASS-MU 26 KDA ISOZYME, DYNEIN HEAVY CHAIN CYTOPLASMIC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	2650	Total	C	N	O	S	0	0	0
			20748	13268	3472	3915	93			
1	B	2650	Total	C	N	O	S	0	0	0
			20748	13268	3472	3915	93			

There are 10 discrepancies between the modelled and reference sequences:

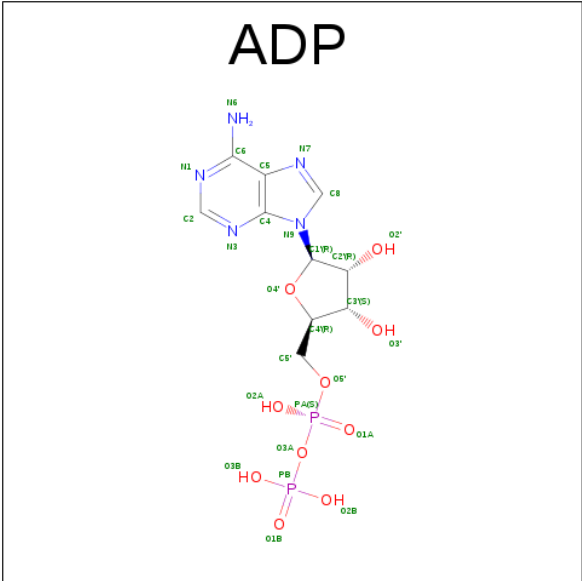
Chain	Residue	Modelled	Actual	Comment	Reference
A	217	LYS	-	LINKER	UNP P36022
A	218	SER	-	LINKER	UNP P36022
A	219	ASP	-	LINKER	UNP P36022
A	1630	ILE	LEU	CONFLICT	UNP P36022
A	3782	ASP	GLU	CONFLICT	UNP P36022
B	217	LYS	-	LINKER	UNP P36022
B	218	SER	-	LINKER	UNP P36022
B	219	ASP	-	LINKER	UNP P36022
B	1630	ILE	LEU	CONFLICT	UNP P36022
B	3782	ASP	GLU	CONFLICT	UNP P36022

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



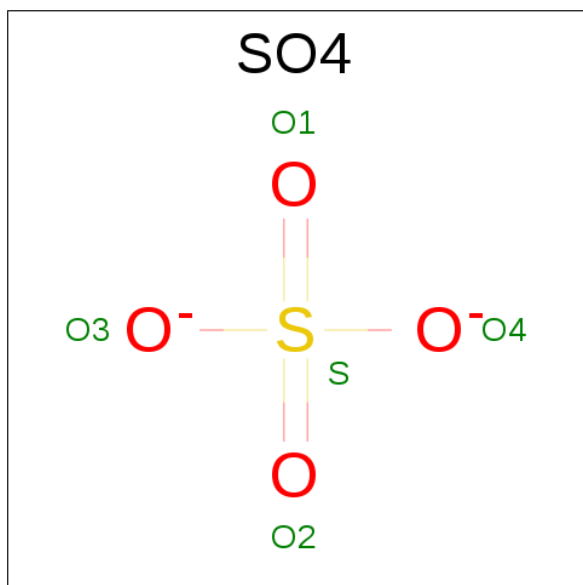
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		

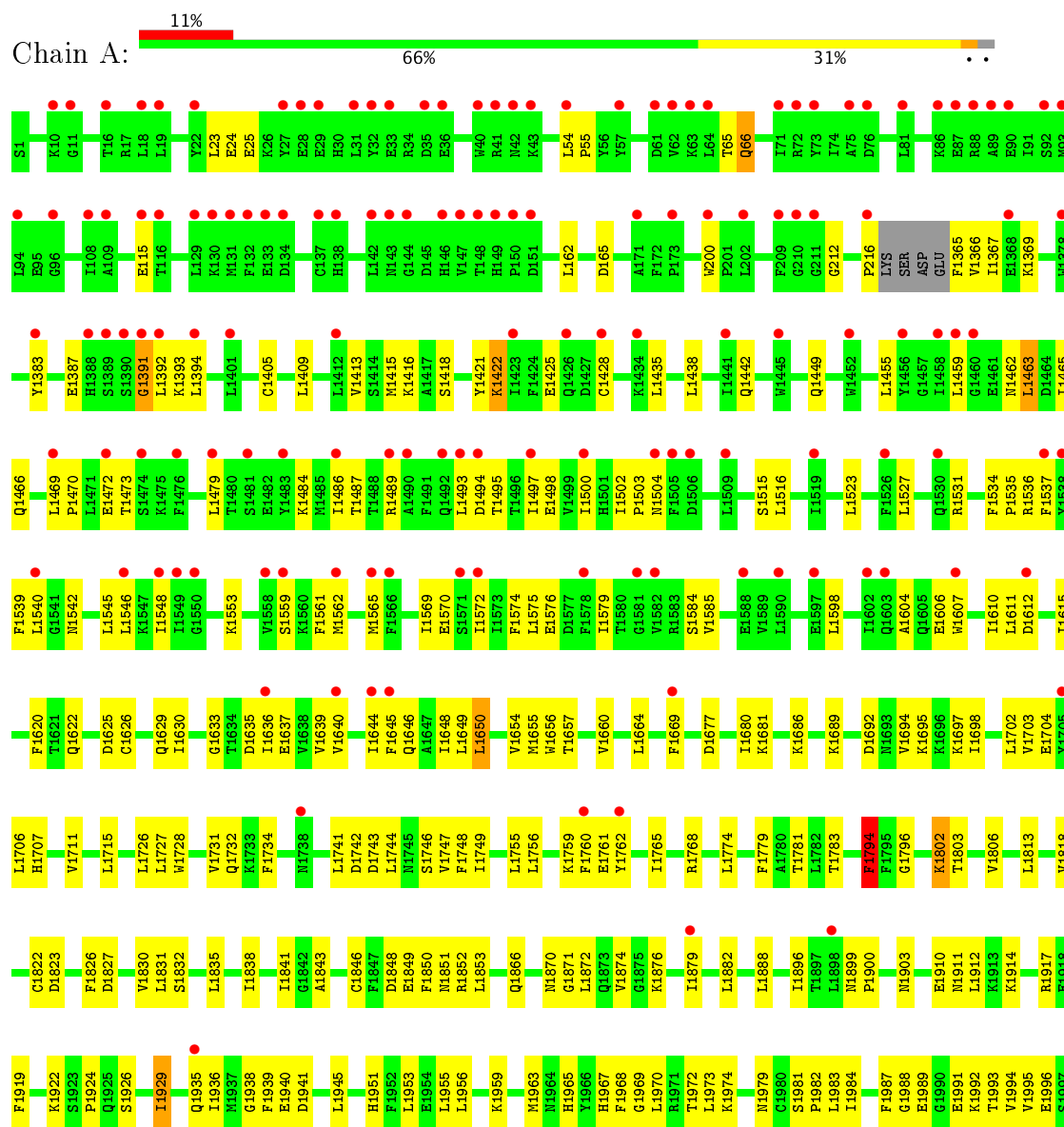
- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Mg	0	0
			1	1		
5	A	1	Total	Mg	0	0
			1	1		

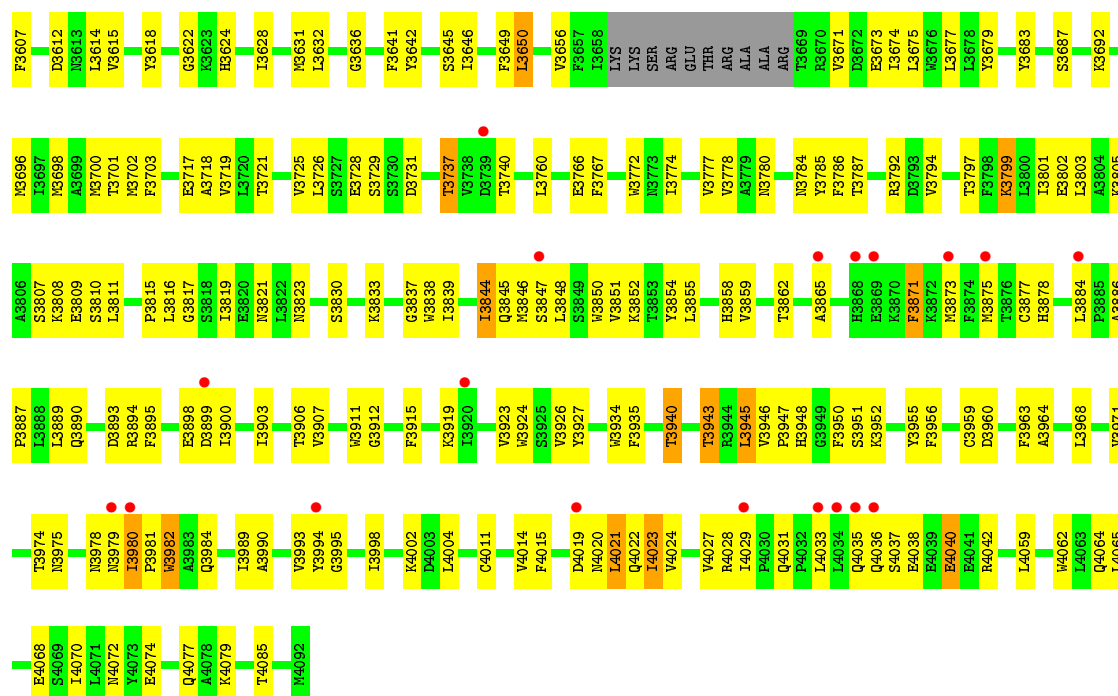
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: GLUTATHIONE S-TRANSFERASE CLASS-MU 26 KDA ISOZYME, DYNEIN HEAVY CHAIN CYTOPLASMIC



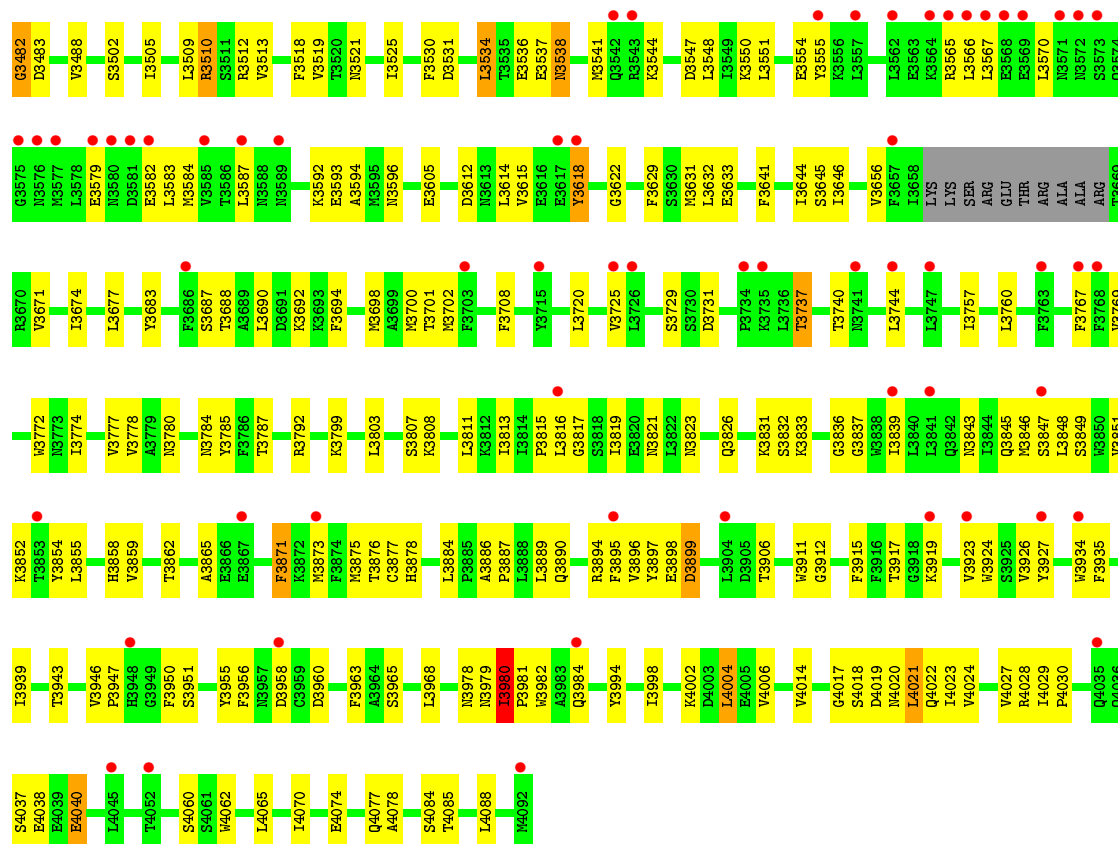
L3534	L3535	E3536	E3537	N3538	N3541	Q3542	R3543	K3544	D3547	L3548	L3549	L3551	E3554	E3555	K3556	K3558	L3559	K3560	K3561	L3562	E3563	K3564	L3565	L3566	L3567	L3570	G3575	N3576	K3577	L3578	E3579	N3580	D3581	E3582	L3583	N3584	L3587	N3588	L3589	L3590	K3591	K3592	E3593	N3594	L3595	N3596	L3597	E3598	L3601																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													
I3408	D3409	I3415	K3425	T3426	F3436	R3439	L3440	F3446	G3447	S3448	F3458	D3459	P3460	I3461	S3462	S3463	R3464	S3467	N3471	H3472	R3476	V3477	V3478	E3480	E3481	I3505	P3506	L3509	R3510	V3513	F3518	V3519	T3520	N3521	I3525	N3526	K3527	L3528	L3529	F3529	L3530	L3531	L3532	L3533	L3534	L3535	L3536	L3537	L3538	L3539	L3540																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																											
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H2886	F2889	T2890	T2891	C2892	P2893	T2894	M2902	L2908	F2909	M2910	L2911	C2912	V2916	H2917	G2918	D2919	M2920	T2924	A2929	V2933	L2936	F2937	M2938	E2939	F2940	T2941	D2942	F2943	ILE	VAL	PRO	GLU	VAL	ASN	THR	LEU	SER	ILE	LEU	SER	VAL	THR	GLU	PRO	GLN	T2960	T2961	R2962	D2963	A2964	V2965																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																											
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I3408	D3409	I3415	K3425	T3426	F3436	R3439	L3440	F3446	G3447	S3448	F3458	D3459	P3460	I3461	S3462	S3463	R3464	S3467	N3471	H3472	R3476	V3477	V3478	E3480	E3481	I3505	P3506	L3509	R3510	V3513	F3518	V3519	T3520	N3521	I3525	N3526	K3527	L3528	L3529	F3529	L3530	L3531	L3532	L3533	L3534	L3535	L3536	L3537	L3538	L3539	L3540																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																											
L1998	K1999	R2000	V2001	L2002	L2003	L2006	F2014	L2021	D2022	E2023	S2024	L2032	A2033	L2034	V2035	L2038	R2039	L2043	Q2044	G2045	G2046	L2047	F2060	Y2061	L2062	M2063	Q2064	R2065	L2066	Q2067	Q2068	A2069	L2070	L2072	L2073	G2074	K2075	A2076	G2077	G2078	G2079	K2080	L2081	L2082	L2083	L2084	K2085																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															
T2086	V2087	L2088	M2091	D2095	M2099	L2104	T2106	K2107	L2108	T2110	K2111	E2112	S2117	A2121	T2122	L2123	E2124	R2125	G2126	G2127	G2128	L2129	F2130	T2131	V2137	L2141	F2145	R2149	L2151	V2152	V2153	F2154	S2156	E2161	L2170	N2173	K2174	L2175	L2176	L2177	P2179	L2180	E2181	L2182	E2183	L2184																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																
Q2185	R2186	T2187	L2188	Q2189	F2190	L2193	D2197	R2201	T2202	T2203	P2204	A2205	R2209	L2212	T2215	V2219	C2220	S2221	L2222	S2223	S2224	R2225	L2226	L2237	D2238	N2239	L2241	L2246	D2247	V2248	L2249	L2252	D2255	F2257	L2262	T2266	L2267	L2268	L2269	L2270	L2271	L2272	L2273	L2274	L2275	L2276	L2277	L2278	L2279	L2280	L2281																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																											
L2282	K2283	L2284	E2285	L2286	A2287	V2288	Q2289	F2290	L2291	E2292	L2293	D2294	L2295	R2299	F2302	Q2303	L2304	L2310	T2314	T2315	L2316	L2317	L2318	S2321	L2322	L2323	L2326	G2332	D2333	R2336	L2339	F2346	S2350	L2353	S2354	D2355	Y2356	S2357	T2358	L2359	V2360	L2361	L2362	L2363	L2364	L2365	L2366	L2367	L2368	L2369	L2370	L2371	L2372	L2373	L2374	L2375	L2376	L2377	L2378	L2379	L2380	L2381	L2382	L2383	L2384	L2385	L2386	L2387	L2388	L2389	L2390	L2391	L2392	L2393	L2394	L2395	L2396	L2397	L2398	L2399	L2400	L2401	L2402	L2403	L2404	L2405	L2406	L2407	L2408	L2409	L2410	L2411	L2412	P2420	G2421	K2424	T2425	M2426	L2427	M2428	A2431	L2432	L2437	N2444	F2445	S2446	K2447	D2448	T2449	N2453	A2455	P2456	T2457	N2458	L2459	R2460	L2461	L2462	L2463	L2464	L2465	L2466	L2467	L2468	L2469	L2470	L2471	L2472	L2473	L2474	L2475	L2476	L2477	L2478	L2479	L2480	L2481	L2482	F2485	E2488	L2489	M2490	L2491	P2492	K2493	L2494	D2495	K2496	Y2497	G2498	S2499	L2506	Q2508	L2509	K2512	Q2513	Q2514	R2517	T2518	P2519	V2524	T2525	L2526	E2527	R2528	A2534	C2535	N2536	R2543	R2549	F2550	L2551	R2552	F2553	D2554	L2555	L2556	L2557	L2558	L2559	L2560	L2561	L2562	S2563	L2564	L2565	L2566	L2567	L2568	L2569	L2570	L2571	Y2574	Y2575	L2576	A2577	L2578	L2581	V2582	F2582	K2589	L2590	L2591	L2592	L2593	L2594	L2595	L2596	L2597	L2598	L2599	L2600	L2601	L2602	L2603	L2604	L2605	L2606	L2607	L2608	L2609	L2610	L2611	L2612	L2613	L2614	L2615	L2616	L2617	L2618	L2619	L2620	L2621	L2622	L2623	L2624	L2625	L2626	L2627	L2628	L2629	L2630	L2631	L2632	L2633	L2634	L2635	L2636	L2637	L2638	Q2639	L2640	S2643	L2644	L2645	L2646	L2647	L2648	L2649	L2650	L2651	L2652	L2653	L2654	L2655	L2656	L2657	L2658	L2659	L2660	L2661	L2662	L2663	L2664	L2665	L2666	L2667	L2668	L2669	L2670	L2671	L2672	L2673	L2674	L2675	L2676	L2677	L2678	L2679	L2680	L2681	L2682	L2683	L2684	L2685	L2686	L2687	L2688	L2689	L2690	L2691	L2692	L2693	L2694	L2695	L2696	L2697	L2698	L2699	L2700	L2701	L2702	L2703	F2704	V2707	N2708	L2712	L2713	L2714	L2715	L2716	L2717	L2718	L2719	L2720	L2721	L2722	L2723	L2724	L2725	L2726	L2727	L2728	L2729	L2730	L2731	L2732	L2733	L2734	L2735	L2736	L2737	L2738	L2739	L2740	L2741	L2742	L2743	L2744	L2745	L2746	L2747	L2748	L2749	L2750	L2751	L2752	L2753	L2754	L2755	L2756	L2757	L2758	L2759	L2760	L2761	L2762	L2763	L2764	L2765	L2766	L2767	L2768	L2769	L2770	L2771	L2772	L2773	L2774	L2775	L2776	L2777	L2778	L2779	L2780	L2781	L2782	L2783	L2784	L2785	L2786	L2787	L2788	L2789	L2790	L2791	L2792	L2793	L2794	L2795	L2796	L2797	L2798	L2799	L2800	L2801	L2802	L2803	L2804	L2805	L2806	L2807	L2808	L2809	L2810	L2811	L2812	L2813	L2814	L2815	L2816	L2817	L2818	L2819	L2820	L2821	L2822	L2823	L2824	L2825	L2826	L2827	L2828	L2829	L2830	L2831	L2832	L2833	L2834	L2835	L2836	L2837	L2838	L2839	L2840	L2841	L2842	L2843	L2844	L2845	L2846	L2847	L2848	L2849	L2850	L2851	L2852	L2853	L2854	L2855	L2856	L2857	L2858	L2859	L2860	L2861	L2862	L2863	L2864	L2865	L2866	L2867	L2868	L2869	L2870	L2871	L2872	L2873	L2874	L2875	L2876	L2877	L2878	L2879	L2880	L2881	L2882	L2883	L2884	L2885	L2886	L2887	L2888	L2889	L2890	L2891	L2892	L2893	L2894	L2895	L2896	L2897	L2898	L2899	L2900	L2901	L2902	L2903	L2904	L2905	L2906	L2907	L2908	L2909	L2910	L2911	L2912	L2913	L2914	L2915	L2916	L2917	L2918	L2919	L2920	L2921	L2922	L2923	L2924	L2925	L2926	L2927	L2928	L2929	L2930	L2931	L2932	L2933	L2934	L2935	L2936	L2937	L2938	L2939	L2940	L2941	L2942	L2943	L2944	L2945	L2946	L2947	L2948	L2949	L2950	L2951	L2952	L2953	L2954	L2955	L2956	L2957	L2958	L2959	L2960	L2961	L2962	L2963	L2964	L2965	L2966	L2967	L2968	L2969	L2970	L2971	L2972	L2973	L2974	L2975	L2976	L2977	L2978	L2979	L2980	L2981	L2982	L2983	L2984	L2985	L2986	L2987	L2988	L2989	L2990	L2991	L2992	L2993	L2994	L2995	L2996	L2997	L2998	L2999	L3000	L3001	L3002	L3003	L3004	L3005	L3006	L3007	L3008	L3009	L3010	L3011	L3012	L3013	L3014	L3015	L3016	L3017	L3018	L3019	L3020	L3021	L3022	L3023	L3024	L3025	L3026	L3027	L3028	L3029	L3030	L3031	L3032	L3033	L3034	L3035	L3036	L3037	L3038	L3039	L3040	L3041	L3042	L3043	L3044	L3045	L3046	L3047	L3048	L3049	L3050	L3051	L3052	L3053	L3054	L3055	L3056	L3057	L3058	L3059	L3060	L3061	L3062	L3063	L3064	L3065	L3066	L3067	L3068	L3069	L3070	L3071	L3072	L3073	L3074	L3075	L3076	L3077	L3078	L3079	L3080	L3081	L3082	L3083	L3084	L3085	L3086	L3087	L3088	L3089	L3090	L3091	L3092	L3093	L3094	L3095	L3096	L3097	L3098	L3099	L3100	L3101	L3102	L3103	L3104	L3105	L3106	L3107	L3108	L3109	L3110	L3111	L3112	L3113	L3114	L3115	L3116	L3117	L3118	L3119	L3120	L3121	L3122	L3123	L3124	L3125	L3126	L3127	L3128	L3129	L3130	L3131	L3132	L3133	L3134	L3135	L3136	L3137	L3138	L3139	L3140	L3141	L3142	L3143	L3144	L3145	L3146	L3147	L3148	L3149	L3150	L3151	L3152	L3153	L3154	L3155	L3156	L3157	L3158	L3159	L3160	L3161	L3162	L3163	L3164	L3165	L3166	L3167	L3168	L3169	L3170	L3171	L3172	L3173	L3174	L3175	L3176	L3177	L3178	L3179	L3180	L3181	L3182	L3183	L3184	L3185	L3186	L3187	L3188	L3189	L3190	L3191	L3192	L3193	L3194	L3195	L3196	L3197	L3198	L3199	L3200	L3201	L3202	L3203	L3204	L3205	L3206	L3207	L3208	L3209	L3210	L3211	L3212	L3213	L3214	L3215	L3216	L3217	L3218	L3219	L3220	L3221	L3222	L3223	L3224	L3225	L3226	L3227	L3228	L3229	L3230	L3231	L3232	L3233	L3234	L3235	L3236	L3237	L3238	L3239	L3240	L3241	L3242	L3243	L3244	L3245	L3246	L3247	L3248	L3249	L3250	L3251	L3252	L3253	L3254	L3255	L3256	L325



• Molecule 1: GLUTATHIONE S-TRANSFERASE CLASS-MU 26 KDA ISOZYME, DYNEIN HEAVY CHAIN CYTOPLASMIC



Y3360	D3361	I3367	V3371	T3372	F3390	L3391	E3392	N3393	S3400	Q3401	D3402	A3403	F3406	L3407	L3408	D3409	H3413	H3414	T3415	V3417	L3429	R3439	L3440	A3443	F3446	V3450	D3459	P3460	I3461	I3462	S3463	L3465	S3466	F3470	N3471	H3472	A3473	R3476	V3477	T3478	I3481											
LEU	VAL	ASN	GLU	LEU	ASN	THR	LEU	VAL	PRO	GLU	VAL	ASN	LYS	GLU	LEU	VAL	PHE	THR	R3303	E3304	R3305	R3306	L3307	N3308	R3311	Q3312	F3313	S3314	F3315	T3316	S3317	E3318	F2972	V2982	Q2983	S2988	P2989	Q2990	K3001	L3010	Q3011	E3012	F3016	N3017	N3018	V3019	G3020	L3024	K3025	E3026	S3027	V3028
E2824	T2825	A2826	E2829	N2832	T2833	L2834	L2835	A2838	D2842	L2843	F2844	Q2845	G2846	Y2849	L2852	L2853	L2856	T2860	L2866	L2867	E2870	L2873	F2877	V2878	H2886	F2889	T2890	L2891	C2892	D2893	P2894	M2902	L2903	A2907	N2910	R2911	L2912	C2912	I2913	L2914	N2915	W2916	L2922	V2923	F2924	L2925	T2926					
W2920	T2924	H2938	T2941	D2942	L2943	ILE	VAL	PRO	GLU	VAL	ASN	LYS	GLU	LEU	VAL	PHE	THR	R3303	E3304	R3305	R3306	L3307	N3308	R3311	Q3312	F3313	S3314	F3315	T3316	S3317	E3318	F2972	V2982	Q2983	S2988	P2989	Q2990	K3001	L3010	Q3011	E3012	F3016	N3017	N3018	V3019	G3020	L3024	K3025	E3026	S3027	V3028	
P2591	L2734	S2737	M2738	H2741	L2742	L2743	L2744	L2745	Q2751	G2754	H2755	M2756	F2757	L2758	L2759	G2760	A2761	R2664	V2663	L2664	R2664	L2673	V2677	L2686	P2562	S2563	S2566	L2694	L2695	L2702	V2707	T2708	K2709	K2580	L2581	L2582	V2582	R2586	S2587	M2732	V2733	L2734	T2735	L2736	L2737	L2738	L2739	L2740				
Y2497	G2498	S2499	L2506	R2507	Q2508	K2512	Q2513	K2517	T2518	P2519	E2520	V2524	T2525	L2526	E2527	L2528	Q2529	H2530	I2531	C2535	N2536	G2542	L2543	L2544	R2549	R2552	H2553	L2556	P2562	S2563	S2566	Y2571	E2572	L2573	Y2574	Y2575	L2578	F2579	K2580	L2581	L2582	V2582	R2586	S2587	E2590							
D2406	N2409	S2410	K2411	R2412	I2415	L2416	C2417	P2420	K2424	T2425	M2428	L2437	V2440	F2445	S2446	K2447	D2448	T2449	L2455	L2458	Y2464	T2467	S2468	L2471	T2472	L2473	L2474	P2475	K2476	S2477	D2478	K2480	L2484	E2488	R2489	R2490	L2491	P2492	K2493	L2494	D2495	K2496										
S2309	L2310	K2311	D2312	V2313	L2314	T2315	L2316	L2317	K2318	R2319	R2320	S2321	L2322	L2326	G2332	Q2335	R2336	I2339	F2346	S2350	Q2351	S2354	S2356	R2355	Y2356	S2357	T2358	L2359	L2361	A2362	N2363	D2364	K2365	L2366	S2367	F2368	V2378	S2379	L2380	E2384	R2385	R2386	R2387	L2390	T2394	L2395	D2396	T2397				
D2197	F2198	L2199	H2201	T2202	T2203	T2204	A2205	L2212	C2220	S2221	T2222	S2223	S2224	K2225	L2229	L2230	N2239	V2261	V2262	K2263	K2264	S2265	F2267	L2268	L2269	L2270	L2271	L2272	L2273	L2274	L2275	L2276	R2279	T2280	F2281	N2282	E2285	V2288	H2293	L2294	L2295	R2299	F2302	L2305	D2306							
L2109	T2110	E2111	S2117	K2121	T2122	L2123	D2127	K2132	T2131	V2137	I2141	F2145	R2149	V2151	V2152	V2153	F2154	D2155	S2156	D2157	L2158	D2159	T2160	E2161	E2164	V2169	D2172	K2174	L2175	L2176	T2177	L2178	G2181	E2182	R2183	T2186	F2190	T2192	L2193	F2194	E2195	T2196										
F1826	D1827	Y1828	Q1829	V1830	H1831	S1832	L1833	L1834	L1835	I1838	I1841	G1842	A1843	G1845	E1849	F1850	N1851	L1852	L1853	V1857	M1864	I1865	Q1866	N1870	G1871	L1872	L1882	L1888	N1889	P1900	R1905	L1908	P1909	E1910	N1911	L1912	R1917	E1918	F1919	S1920	M1921	K1922	S1923	Q1924	S1926							
I1929	Q1935	H1936	H1937	G1938	F1939	E1940	D1941	S1942	L1945	I1949	F1952	L1953	L1956	H1967	F1968	G1969	L1970	R1971	T1972	L1973	K1974	L1977	R1978	L1979	P1980	S1981	P1982	L1983	L1984	E1989	G1990	E1991	K1992	T1993	V1994	V1995	E1996	S1997	L1998	K1999	R2000	V2001	T2002	L2003	M2006	G2007	D2008	E2011				
F2014	T2021	D2023	S2024	T2027	P2028	K2032	L2034	V2035	G2042	D2043	R2044	P2049	F2060	V2061	V2062	K2063	K2064	T2065	T2066	D2067	K2068	K2069	L2070	L2071	L2072	V2073	G2074	K2080	T2081	A2082	T2083	K2084	K2085	T2086	V2087	T2088	M2091	K2092	T2093	F2094	D2095	M2099	D2105	T2106	V2108							



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	174.89Å 119.17Å 193.97Å 90.00° 90.18° 90.00°	Depositor
Resolution (Å)	49.29 – 3.40 49.24 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.29-3.40) 99.9 (49.24-3.40)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.35 (at 3.40Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.241 , 0.303 0.236 , 0.300	Depositor DCC
R_{free} test set	5512 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	133.4	Xtriage
Anisotropy	0.397	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 132.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.033 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	41678	wwPDB-VP
Average B, all atoms (Å ²)	190.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.79% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, MG, SO4, ADP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.54	0/21146	0.77	12/28618 (0.0%)
1	B	0.52	0/21146	0.76	9/28618 (0.0%)
All	All	0.53	0/42292	0.77	21/57236 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	2455	LEU	CB-CG-CD1	-8.01	97.38	111.00
1	A	3650	LEU	CB-CG-CD1	-7.07	98.98	111.00
1	A	1882	LEU	CA-CB-CG	6.87	131.09	115.30
1	A	1463	LEU	CA-CB-CG	6.63	130.55	115.30
1	A	3945	LEU	CB-CG-CD2	-6.48	99.98	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	3308	ASN	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	20748	0	20206	934	0
1	B	20748	0	20207	930	0
2	A	31	0	12	6	0
2	B	31	0	12	22	0
3	A	54	0	24	28	0
3	B	54	0	24	29	0
4	A	5	0	0	2	0
4	B	5	0	0	2	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
All	All	41678	0	40485	1867	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 23.

The worst 5 of 1867 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2732:MET:HB2	3:B:5402:ADP:C6	1.40	1.57
1:B:1365:PHE:CD1	1:B:1366:VAL:HG23	1.34	1.57
1:A:1365:PHE:CE2	1:A:1366:VAL:HG23	1.55	1.39
1:A:1365:PHE:CD2	1:A:1366:VAL:HG23	1.68	1.27
1:B:1365:PHE:CE1	1:B:1366:VAL:HG23	1.70	1.27

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	2640/2695 (98%)	2503 (95%)	121 (5%)	16 (1%)	28 68
1	B	2640/2695 (98%)	2506 (95%)	116 (4%)	18 (1%)	25 65
All	All	5280/5390 (98%)	5009 (95%)	237 (4%)	34 (1%)	28 68

5 of 34 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	24	GLU
1	A	1391	GLY
1	A	2369	SER
1	A	3309	THR
1	B	1391	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	2218/2453 (90%)	2128 (96%)	90 (4%)	35 71
1	B	2218/2453 (90%)	2133 (96%)	85 (4%)	38 72
All	All	4436/4906 (90%)	4261 (96%)	175 (4%)	37 72

5 of 175 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3900	ILE
1	B	1525	THR
1	B	3831	LYS
1	A	3940	THR
1	A	4064	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 65 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3685	GLN
1	B	1501	HIS
1	B	3783	ASN
1	A	3780	ASN
1	A	4031	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	ATP	A	5400	-	27,33,33	1.01	1 (3%)	25,52,52	1.66	2 (8%)
3	ADP	A	5401	-	25,29,29	1.22	2 (8%)	24,45,45	1.57	4 (16%)
3	ADP	A	5402	-	25,29,29	1.03	1 (4%)	24,45,45	1.93	3 (12%)
4	SO4	A	5403	-	4,4,4	0.43	0	6,6,6	0.71	0
2	ATP	B	5400	-	27,33,33	1.01	1 (3%)	25,52,52	1.66	3 (12%)
3	ADP	B	5401	-	25,29,29	1.22	1 (4%)	24,45,45	1.90	4 (16%)
3	ADP	B	5402	-	25,29,29	1.00	1 (4%)	24,45,45	1.73	3 (12%)
4	SO4	B	5403	-	4,4,4	0.42	0	6,6,6	0.44	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ATP	A	5400	-	-	0/18/38/38	0/3/3/3
3	ADP	A	5401	-	-	0/12/32/32	0/3/3/3
3	ADP	A	5402	-	-	0/12/32/32	0/3/3/3
4	SO4	A	5403	-	-	0/0/0/0	0/0/0/0
2	ATP	B	5400	-	-	0/18/38/38	0/3/3/3
3	ADP	B	5401	-	-	0/12/32/32	0/3/3/3
3	ADP	B	5402	-	-	0/12/32/32	0/3/3/3
4	SO4	B	5403	-	-	0/0/0/0	0/0/0/0

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	5401	ADP	C2-N3	2.54	1.36	1.32
2	A	5400	ATP	C5-C4	2.99	1.47	1.40
3	A	5402	ADP	C5-C4	3.03	1.47	1.40
2	B	5400	ATP	C5-C4	3.07	1.47	1.40
3	B	5402	ADP	C5-C4	3.24	1.47	1.40

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	5402	ADP	N3-C2-N1	-7.17	122.61	128.86
3	B	5401	ADP	N3-C2-N1	-6.89	122.86	128.86
3	B	5402	ADP	N3-C2-N1	-6.41	123.28	128.86
2	B	5400	ATP	N3-C2-N1	-5.84	123.77	128.86
2	A	5400	ATP	N3-C2-N1	-5.80	123.80	128.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 89 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	5400	ATP	6	0
3	A	5401	ADP	11	0
3	A	5402	ADP	17	0
4	A	5403	SO4	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	5400	ATP	22	0
3	B	5401	ADP	6	0
3	B	5402	ADP	23	0
4	B	5403	SO4	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	2650/2695 (98%)	0.60	298 (11%) 6 6	88, 185, 310, 500	1 (0%)
1	B	2650/2695 (98%)	0.70	256 (9%) 8 9	96, 180, 317, 500	1 (0%)
All	All	5300/5390 (98%)	0.65	554 (10%) 7 7	88, 183, 311, 500	2 (0%)

The worst 5 of 554 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	49	LEU	35.5
1	B	33	GLU	29.8
1	B	83	GLY	27.1
1	B	69	ALA	26.7
1	A	131	MET	24.8

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	MG	B	5404	1/1	0.90	0.30	1.51	107,107,107,107	0
2	ATP	A	5400	31/31	0.94	0.31	1.08	122,147,224,246	0
4	SO4	A	5403	5/5	0.92	0.23	0.70	101,136,142,145	0
2	ATP	B	5400	31/31	0.91	0.27	0.62	124,160,195,221	0
3	ADP	B	5401	27/27	0.94	0.27	0.39	98,121,138,153	0
3	ADP	B	5402	27/27	0.87	0.33	0.34	108,145,183,194	0
3	ADP	A	5401	27/27	0.89	0.28	-0.18	126,146,191,198	0
3	ADP	A	5402	27/27	0.93	0.25	-0.69	134,176,208,218	0
4	SO4	B	5403	5/5	0.91	0.16	-0.78	139,143,171,171	0
5	MG	A	5404	1/1	0.77	0.17	-2.20	97,97,97,97	0

6.5 Other polymers [i](#)

There are no such residues in this entry.